# How can ACTS work for you?

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# What is the ACTS Toolkit?

**http://acts.nersc.gov**

- Advanced Computational Testing and Simulation
- Tools for development of (complex) scientific applications
  - (currently) 21 tools
  - developed (primarily) at DOE labs
  - originally conceived as autonomous tools
- ACTS is an “umbrella” project
  - collect tools
  - leverage numerous independently funded projects

# ACTS Project Goals

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- Bring software packages together into a “toolkit”
- Make the software interoperable
- Provide consistent application interfaces
- Promote general solutions to complex programming needs
- Promote code reusability
- Enable large scale applications

# How can ACTS work for you?

- Some examples in computational sciences.
- Which tool? What approach? What do you get?
- A few scientific applications using ACTS Tools.
- Why do we need these tools?
- ACTS services provided at NERSC.
- Our agenda for the Workshop.

***Data***:

$n$ temperature measurements $t_i$ at depths $z_i$ in the Earth

***Goal***:

define a model assuming a quadratic variation of temperature with depth

$$
\begin{aligned}
t_1 &= a + bz_1 + cz_1^2 \\
t_2 &= a + bz_2 + cz_2^2 \\
&\vdots \\
t_n &= a + bz_n + cz_n^2
\end{aligned}
\quad \longrightarrow \quad
\begin{Bmatrix} t_1 \\ t_2 \\ \vdots \\ t_n \end{Bmatrix}
=
\begin{bmatrix} 1 & z_1 & z_1^2 \\ 1 & z_2 & z_2^2 \\ & \vdots & \\ 1 & z_n & z_n^2 \end{bmatrix}
\begin{Bmatrix} a \\ b \\ c \end{Bmatrix}
$$

# A More Realistic Model...

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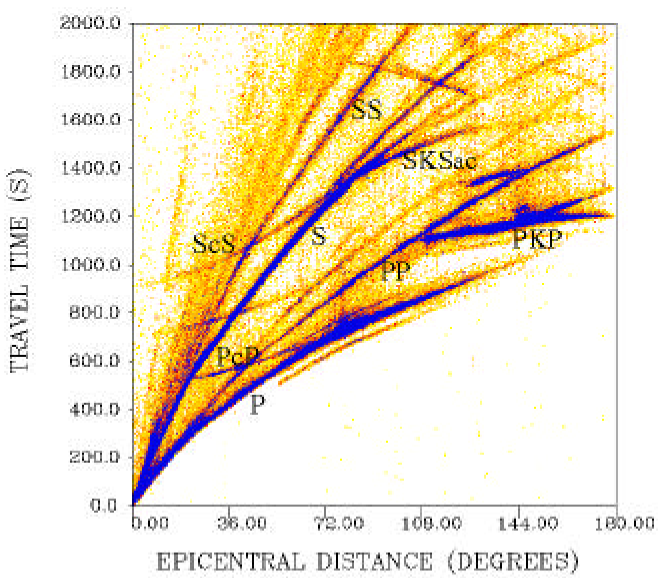
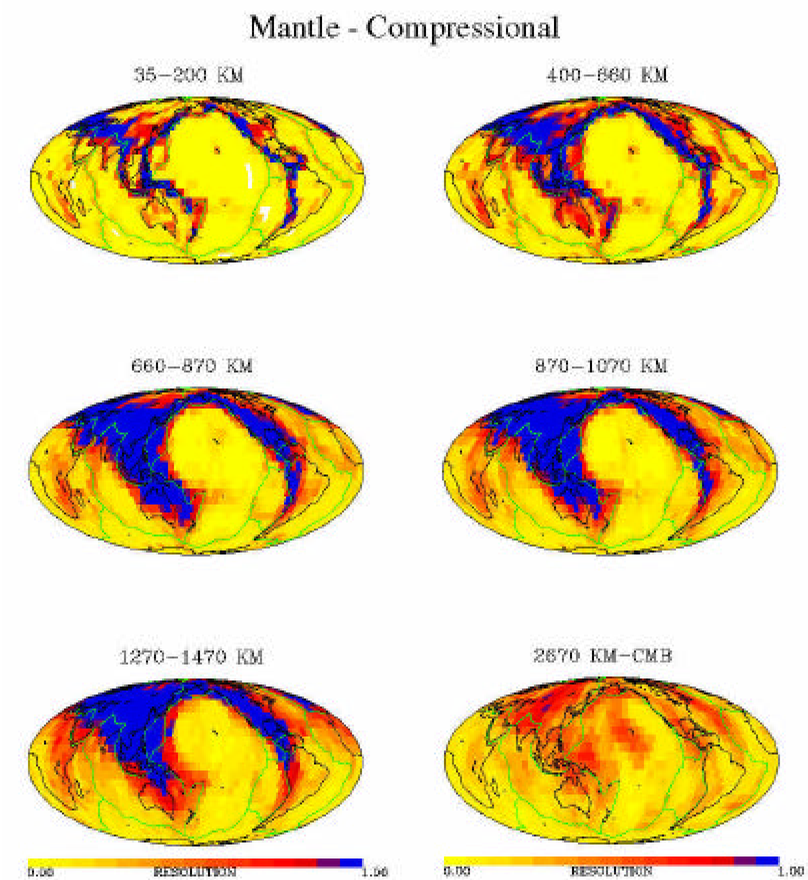
*Travel times of sound waves generated by earthquakes used to infer structure in the entire Earth (crust, mantle and core).*



# Simple Problem: *Poisson's Equation in 1D*

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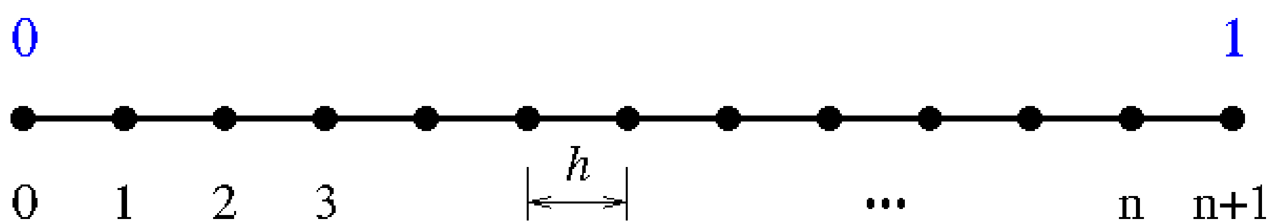
$$-\frac{d^2 v(x)}{dx^2} = f(x), \quad 0 < x < 1$$

$$v(0) = v(1) = 0 \quad (\textit{Dirichlet})$$



# Simple Problem: *Poisson's Equation in 1D*

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## *Centered Finite Difference Approximation:*

$$\frac{dv(x)}{dx}\Big|_{x=(i-\frac{1}{2})h} \approx \frac{v_i - v_{i-1}}{h}$$

$$\frac{dv(x)}{dx}\Big|_{x=(i+\frac{1}{2})h} \approx \frac{v_{i+1} - v_i}{h}$$

$$\rightarrow \quad -\frac{d^2v(x)}{dx^2}\Big|_{x=x_i} \approx \frac{2v_i - v_{i-1} - v_{i+1}}{h^2}$$

$$\text{at point i}: \; -v_{i-1} + 2v_i - v_{i+1} = h^2 f_i$$

$$\begin{bmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{bmatrix} \begin{Bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{Bmatrix} = h^2 \begin{Bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{Bmatrix}$$

# More Realistic Applications...

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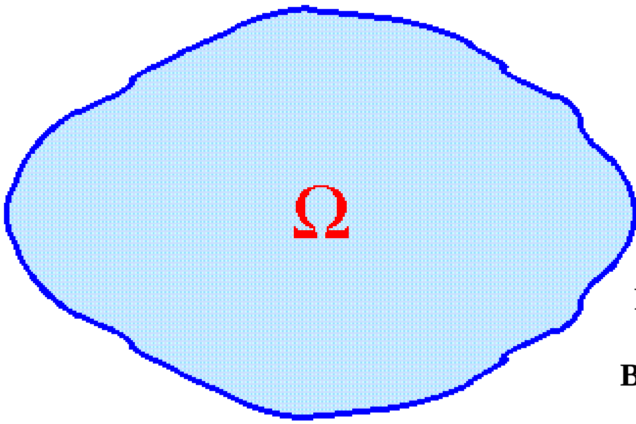
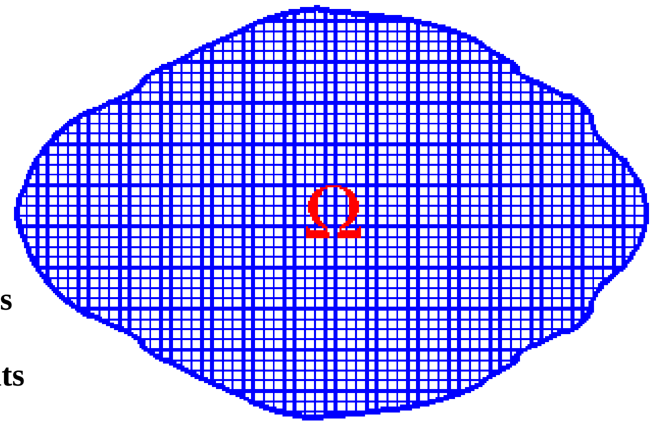
continuous problem




grid →

**Finite Differences**
**Finite Elements**
**Boundary Elements**
**Fourier**
⋮

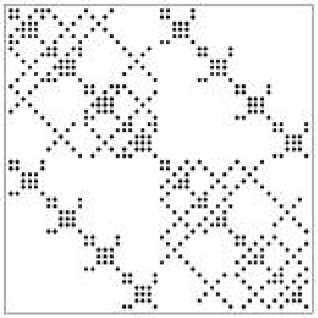
discrete problem




$$m\frac{d^2x}{dt^2} + c\frac{dx}{dt} + kx = f(t)$$

$$\frac{\partial v}{\partial t} = -v\frac{\partial v}{\partial x} + \Gamma\frac{\partial^2 v}{\partial x^2}$$

$$\vdots$$

 $= A$

(sparse matrix)

# Another application: *Motions of Proteins*

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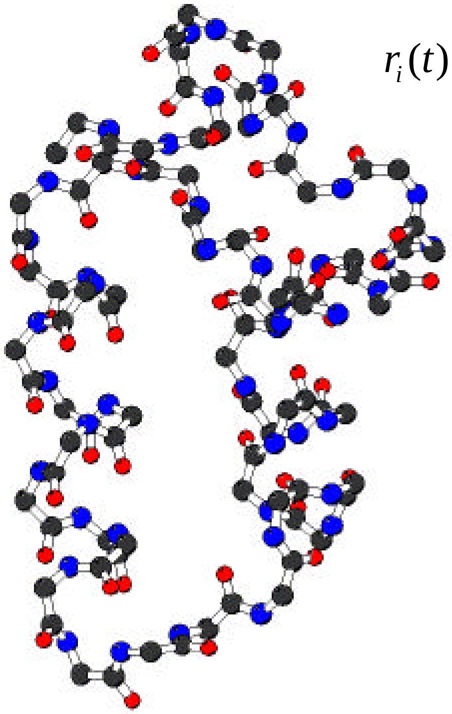
$$V = \frac{1}{2}\sum_{i=1}^{3n}\sum_{j=1}^{3n} k_{ij}(r_i - r_i^s)(r_j - r_j^s)$$

$$r_i(t) = r_i^s + \frac{1}{\sqrt{m_i}}\sum_{j=1}^{3n} a_{ij} q_j(t), \quad i = 1,2,\ldots 3n$$

$$q_j(t) = C_j \cos(\omega_j t + \phi_j)$$



$$A = M^{-\frac{1}{2}}(\nabla^2 E)M^{-\frac{1}{2}}$$

(sparse matrix)

# What needs to be computed?

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$$Ax = b$$

(system of linear equations)

Direct Methods:

1. $A = LU$ ($L$ lower triangular, $U$ upper triangular)
2. $Ly = b$
3. $Ux = y$

SuperLU
ScaLAPACK

Iterative Methods:

$$x_k = x_{k-1} + \alpha_k p_{k-1}$$

only matrix - vector multiplies are needed

preconditoning is usually required

Aztec/Trilinos
Hypre
PETSc

# What needs to be computed?

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$$Az = \lambda z$$

(eigenvalue problem)

ScaLAPACK

$$A = U \Sigma V^T$$

(singular value decomposition)

ScaLAPACK

$$\min \left\{ \tfrac{1}{2} \| r(x) \|^2 : x_l \le x \le x_u \right\}$$

(systems of nonlinear equations)

PETSc
TAO

PDEs

PETSc

$\vdots$

# Other services may also be needed...

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- Computational steering
- Interactive visualization
- Distributed computation
- Data distribution and management
- Performance analysis
- Scripting Languages

  ⋮

Globus
CUMULVS
TAU
Global Arrays
PAWS
SILOON
PADRE

# Usage of ACTS Tools: *ScaLAPACK*

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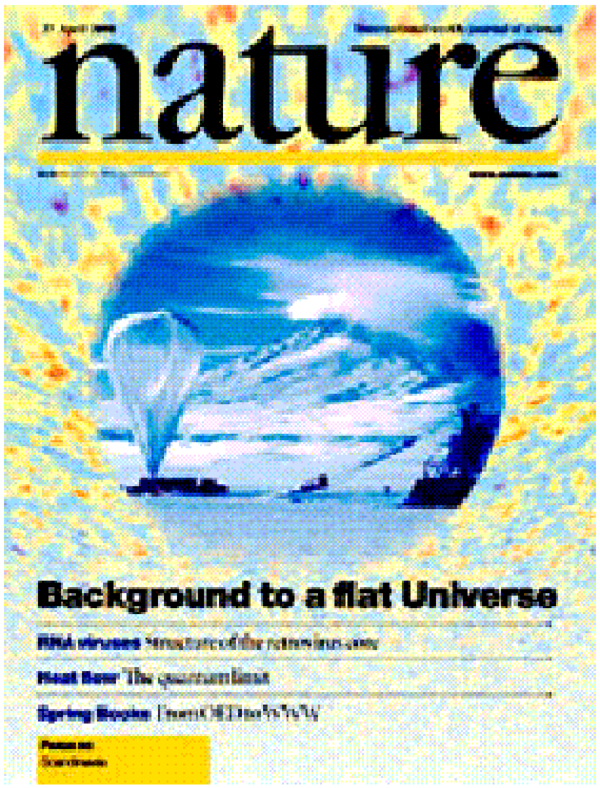


*The international BOOMERanG collaboration announced results of the most detailed measurement of the cosmic microwave background radiation (CMB), which strongly indicated that the universe is flat (Apr. 27, 2000). Likelihood methods implemented in the MADCAP software package were used to examine the large dataset generated by BOOMERanG.*

# Usage of ACTS Tools: *SuperLU*

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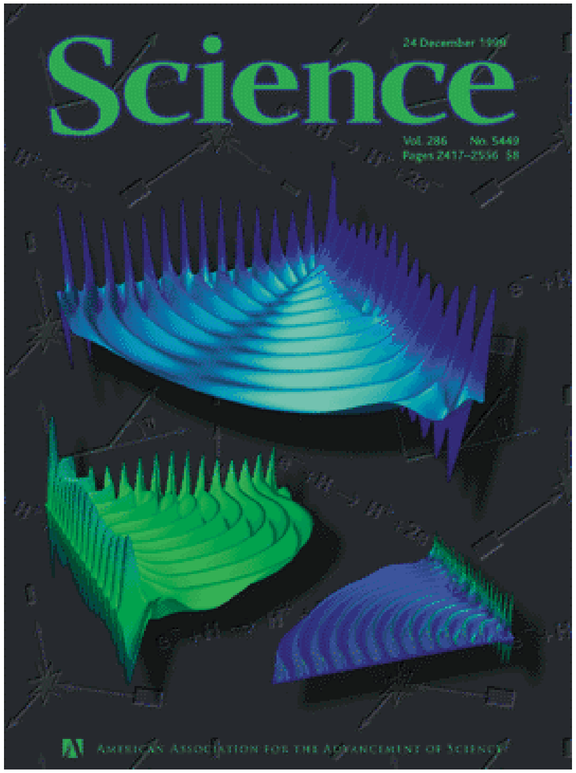


*Collaborators at the Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, and the University of California at Davis have obtained a complete solution of the ionization of a hydrogen atom by collision with an electron, the simplest nontrivial example of the long-standing unsolved problem of scattering in a quantum system of three charge particles. The images show representative wave functions of the problem (Rescigno, Baertschy, Isaacs and McCurdy, Dec. 24, 1999).*

# Usage of ACTS Tools: *Aztec*

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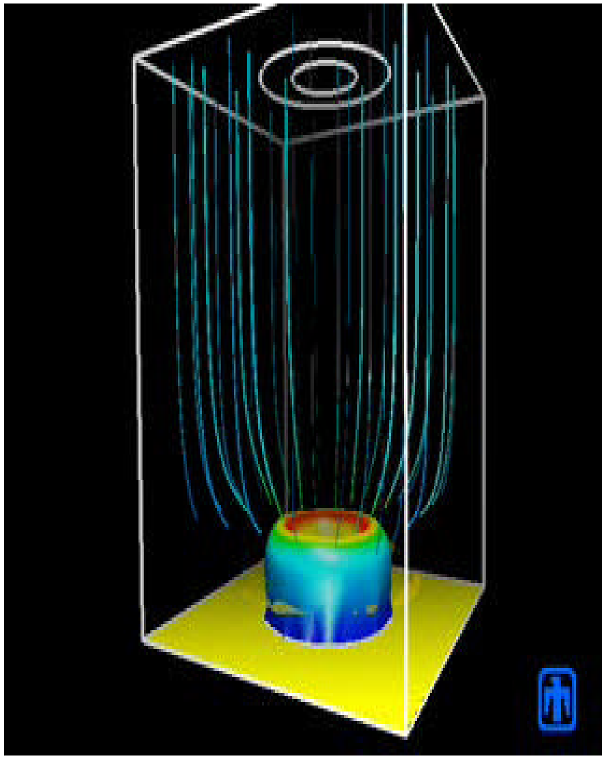

*Co-flowing Annular Jet Combuster. A parallel 3D pseudo-transient simulation to steady state operation. The isosurfaces are of constant velocity in the outflow (z) direction. Four regions of recirculation are shown near corners of solid walls. Isosurfaces are colored by local temperature.*

# Usage of ACTS Tools: *PETSc*

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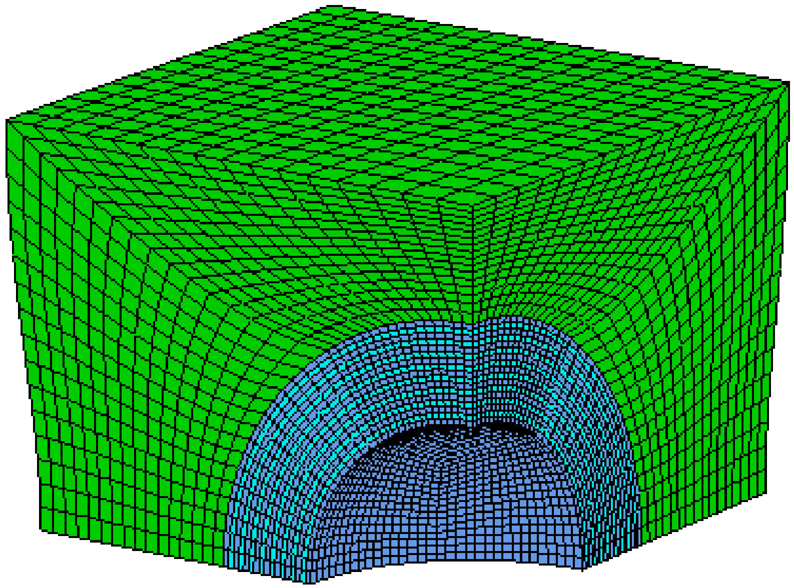

*Prometheus code (unstructured meshes in solid mechanics), parameterized mesh of a "hard" sphere included in a "soft" material. The model shown has 26 million DOF (Adams and Demmel).*

# Why do we need these tools?

- High Performance Tools:
  - portable
  - library calls
  - fault tolerant
  - robust algorithms
  - help code optimization
- More code development in less time
- More simulation in less computer time

# ACTS@NERSC

**http://acts.nersc.gov**

- Make ACTS tools available on NERSC platforms
- Provide technical support
- Perform independent evaluation of tools
- Maintain online ACTS information center
- Identify new users who can benefit from toolkit
- Work with users to integrate tools into applications
- Minimize risk to users

**acts-support@nersc.gov**
**http://acts.nersc.gov**

# Workshop Agenda

- Thursday: numerical tools (ScaLAPACK, SuperLU, Hypre, etc), applications.
- Friday: computational/numerical tools (PETSc and TAO), applications.
- Saturday: development/infrastructure tools (Globus, TAU, CUMULVS, etc).
- ACTS is more than what we will be able to cover in the next three days!